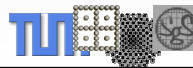


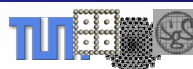
## Tools: Libraries and Software

- In addition to standard tools like editors, compilers, or debuggers, there is a lot of (commercial or public domain) support available:
  - **Modelling:** Computer algebra programs like Mathematica, Maple, Axiom, or Reduce support derivations and proofs of theorems via symbolic means.
  - **Numerics:** Mathematica, Maple, or MATLAB support the development, testing, and analysis of (numerical) algorithms and allow an efficient prototyping.
  - **Implementation:** A zoo of (numerical) libraries provide up-to-date modules for standard tasks (numerical linear algebra etc.), tailored to specific target architectures.
  - **Visualization:** Packages like IDL, IRIS Explorer, or AVS/Express offer (nearly) all you want.



## Libraries and Collections

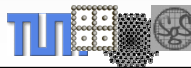
- **GAMS: Guide to Available Mathematical Software**
  - service offered by the National Institute of Standards & Technology (NIST)
  - see <http://gams.nist.gov>
  - catalogue and database of more than 100 packages and libraries with together several tens of thousands of routines
  - Topics range from number theory to statistics!
  - majority: FORTRAN programs for numerical tasks (systems of linear equations, eigenvalues, roots, differential equations, ...)
  - includes both public domain material (at NIST or at NETLIB, see below) and commercial (licenced) products
  - good user guidance



## Libraries and Collections

### ➤ Matrix Market:

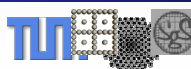
- see <http://math.nist.gov/MatrixMarket/>
- repository of test data for use in comparative studies of algorithms for numerical linear algebra
- features nearly 500 (sparse) matrices from various fields of applications (chemical engineering, fluid flow, power system networks, quantum physics, or structural engineering, e.g.)
- provides also matrix generation tools
- classification according to matrix properties:
  - number field: real or complex
  - nonzero structure: dense, banded, sparse, tridiagonal, ...
  - symmetry: none, symmetric, skew symmetric, SPD, SPSP, ...
  - shape: square, more rows than columns, ...



## Libraries and Collections

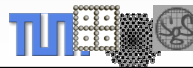
### ➤ NETLIB: repository of free software for numerical purposes

- see <http://www.netlib.org/>
- offered by University of Tennessee and Oak Ridge Nat'l Lab
- several mirrored copies all over the world
- about 135 million requests since 1985, > 40 million in 2000
- > 90% http, rest ftp and email
- about 160 different libraries, among which
  - BLAS (Basic Linear Algebra Subprograms)
  - LAPACK (Linear Algebra PACKage)
  - ODEPACK (ordinary differential equations)
  - MPI (message passing interface for parallelization)
  - PLTMG (elliptic boundary value problems)



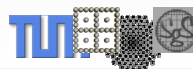
## BLAS

- collection of robust, efficient, and portable modules for elementary vector and matrix operations
- basis for LAPACK routines, for example
- allows plug-and-play for numerical subroutines
- FORTRAN, to be used from FORTRAN/C/C++
- Java BLAS available, too
- levels:
  - **Level 1:** vector and vector-vector operations (norm, scalar product, vector addition, SAXPY, ...)
  - **Level 2:** matrix-vector operations (rank-1-modifications, matrix-vector product, tridiagonal systems); vector processors
  - **Level 3:** matrix-matrix operations; parallel computers!



## LAPACK

- popular collection of FORTRAN subroutines for standard problems from numerical linear algebra like linear systems, regression, eigenvalues, SVD, ...
- dense and band matrices (not general sparse ones)
- successor of EISPACK and LINPACK, tuning for modern microprocessors and supercomputer architectures (reduction of memory accesses, block operations, ...)
- LAPACK routines use BLAS modules
- variants:
  - LAPACK90, CLAPACK, LAPACK++
  - ScaLAPACK (MIMD systems, scalability!)

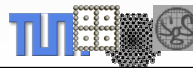


## Libraries and Collections

- Visual Numerics:
  - see <http://www.vni.com>
  - mathematical libraries
  - predecessor: IMSL (The Int'l Math. & Statist. Library)
- Diffpack:
  - offered by Numerical Objects, see <http://www.nobjects.com>
  - environment for the development of code for numerical simulation problems plus libraries of efficient routines
  - object-oriented concept, available for most UNIX platforms
- NAG (Numerical Algorithms Group):
  - see <http://www.nag.co.uk/>
  - non-profit software house, spin-off of Oxford University
  - FORTRAN/FORTRAN90/C/Parallel libraries;
  - AXIOM; IRIS Explorer (Visual.); Fastflo (CFD and more)



Introduction to Scientific Computing  
Lesson 2: Tools



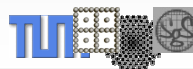
Slide 7

## Libraries and Collections

- Numerical Recipes:
  - see <http://www.nr.com>
  - book series *The Art of Scientific Computing* (CU Press)
  - sophisticated algorithms and their implementations
  - available for FORTRAN 77, FORTRAN 90, C, Pascal, ...
  - corresponding software is licenced and commercial
  - about 350 routines for topics like
    - solution of linear systems
    - interpolation and extrapolation
    - numerical quadrature
    - differentiation and approximation
    - roots and extrema
    - eigenvalues, differential equations, and more



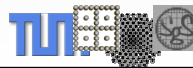
Introduction to Scientific Computing  
Lesson 2: Tools



Slide 8

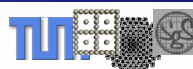
## Tools for Algorithm Development

- Libraries offer tested and efficient (w.r.t. both storage and runtime) standard modules for competitive simulation codes (*do something classical cheap!*)
- Another problem is algorithm development (*develop something new and cheaper!*):
  - design of algorithms
  - testing and rapid prototyping
  - analysis (convergence behaviour etc.)
  - not yet: production runs, memory or runtime optimization
- widespread solutions:
  - computer algebra programs like Maple or Mathematica
  - MATLAB



## Maple

- by Waterloo Maple Inc., a spin-off of the University of Waterloo in Ontario (see <http://www.maplesoft.com>)
- originally a mere computer algebra program, today „interactive environment for mathematical problem solving and programming“
- focus:
  - symbolic computations, formula manipulation
  - numerical computations with arbitrary accuracy
  - 2D and 3D graphical output
  - straightforward programming for algorithm development
- structure:  
kernel + main library + mixed library + packages



# MATLAB

- by The MathWorks (see <http://www.mathworks.com/>)
- originally: primarily for use in (maths) education
- today: „high-performance numerical computation and visualization software“, standard tool for scientific computing research groups:
  - development, prototyping, programming
  - computations
  - visualization
- singular success story: >500 employees, >100 countries, >2000 universities and research institutes
- structure: basic program plus a collection of specialized tool boxes

